Fourier-Optics Compatible Radiation Propagation Methods Used in SRW

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U.S. DEPARTMENT OF ENERGY

BROOKHAVEN NATIONAL LABORATORY
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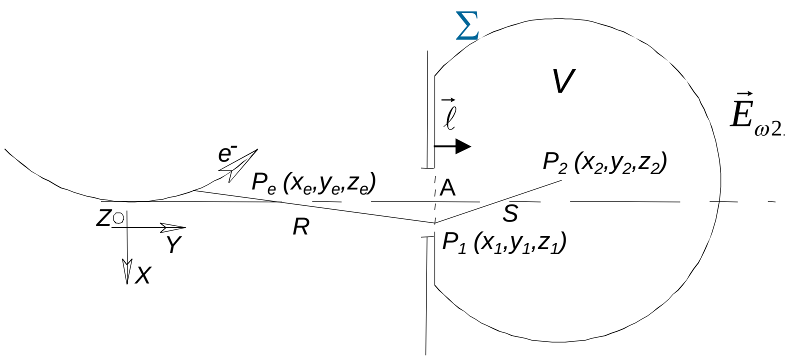
Wavefront Propagation in the Case of Full Transverse Coherence

Kirchhoff Integral Theorem applied to Spontaneous Emission by One Electron



$$\vec{E}_{\omega 2\perp}(P_2) \approx \frac{k^2 e}{4\pi}\int_{-\infty}^{+\infty} d\tau \iint_{A} \frac{\vec{\beta}_{e\perp} - \vec{n}_{\perp}}{RS} \exp[ik(c\tau + R + S)] \cdot (\vec{\ell}\cdot\vec{n}_{p_e p_1} + \vec{\ell}\cdot\vec{n}_{p_1 p_2}) d\Sigma$$

Valid at large observation angles;
Is applicable to complicated cases of diffraction inside vacuum chamber

Huygens-Fresnel Principle

$$\vec{E}_{\omega 2\perp}(P_2) \approx \frac{k}{4\pi i}\iint_{A} \vec{E}_{\omega 1\perp}(P_1) \frac{\exp(ikS)}{S} (\vec{\ell}\cdot\tilde{\vec{n}} + \vec{\ell}\cdot\vec{n}_{p_1 p_2}) d\Sigma$$

Fourier Optics

Free Space:
(between parallel planes perpendicular to optical axis)

$$\vec{E}_{\omega 2\perp}(x_2, y_2) \approx \frac{k}{2\pi i L}\iint \vec{E}_{\omega 1\perp}(x_1, y_1) \exp[ik[L^2 + (x_2 - x_1)^2 + (y_2 - y_1)^2]^{1/2}] dx_1 dy_1$$

Assumption of small angles

"**Thin**" Optical Element:

$$\vec{E}_{\omega 2\perp}(x, y) \approx \mathbf{T}(x, y, \omega)\, \vec{E}_{\omega 1\perp}(x, y)$$

"**Thick**" Optical Element:
(propagation from transverse plane before the element to a transverse plane just after it)

$$\vec{E}_{\omega 2\perp}(x_2, y_2) \approx \mathbf{G}(x_2, y_2, \omega) \exp[ik\Lambda(x_2, y_2, k)]\, \vec{E}_{\omega 1\perp}(x_1(x_2, y_2), y_1(x_2, y_2))$$

Implemented in SRW for Python in 2012;
Currently used for simulation of NSLS-II PX and spectral microscopy beamlines
Benchmarking against experimental data is required

Approach to High-Accuracy Partially-Coherent Emission and Wavefront Propagation Simulations

Averaging (over **phase-space volume** occupied by **e-beam**) of the **intensity** (or mutual intensity, or mathematical brightness) obtained from **electric field emitted by an electron** and **propagated** through an optical system:

$$I_\omega(x,y)=\int I_{\omega 1}(x,y;x_e,y_e,z_e,x'_e,y'_e,\delta\gamma_e)\, f(x_e,y_e,z_e,x'_e,y'_e,\delta\gamma_e)\, dx_e dy_e dz_e dx'_e dy'_e d\delta\gamma_e$$

$$I_{\omega 1}(x,y;x_e,y_e,z_e,x'_e,y'_e,\delta\gamma_e)=\left|\mathbf{E}_{\omega 1\perp}(x,y;x_e,y_e,z_e,x'_e,y'_e,\delta\gamma_e)\right|^2$$

$$M_{\omega 1}(x,y,\tilde{x},\tilde{y};x_e,y_e,z_e,x'_e,y'_e,\delta\gamma_e)=\mathbf{E}_{\omega 1\perp}(x,y;\ x_e,y_e,z_e,x'_e,y'_e,\delta\gamma_e)\mathbf{E}^*_{\omega 1\perp}(\tilde{x},\tilde{y};\ x_e,y_e,z_e,x'_e,y'_e,\delta\gamma_e)$$

$$B_{\omega 1}(x,y,\theta_x,\theta_y;x_e,y_e,z_e,x'_e,y'_e,\delta\gamma_e)\sim\mathbf{E}_{\omega 1\perp}(x,y;\ x_e,y_e,z_e,x'_e,y'_e,\delta\gamma_e)\int\mathbf{E}^*_{\omega 1\perp}(\tilde{x},\tilde{y};\ x_e,y_e,z_e,x'_e,y'_e,\delta\gamma_e)\exp\left[i\frac{\omega}{c}(\theta_x\tilde{x}+\theta_y\tilde{y})\right]d\tilde{x}d\tilde{y}$$

This method is **general** and **accurate**. For the most part, it is already implemented in SRW code. However, it can be **CPU-intensive**, requiring **parallel calculations** on a multi-core server or a small cluster. Several approaches are considered for increasing the efficiency, including use of low-discrepancy sequences (collaboration with R. Lindberg, K.-J. Kim, X. Shi, ANL), “improved Monte-Carlo” type techniques, as well as “coherent mode decomposition”.

NOTE: the **smaller** the **e-beam emittance** (the higher the radiation coherence) – the **faster** is the **convergence** of simulations with this general method.

NOTE: **convolution** can be valid in some cases, such as pure projection geometry, focusing by a thin lens, diffraction at one slit, etc.

$$I_\omega(x,y)\approx\int\tilde{I}_{\omega 1}(x-\tilde{x}_e,y-\tilde{y}_e)\,\tilde{f}(\tilde{x}_e,\tilde{y}_e)\,d\tilde{x}_e d\tilde{y}_e$$

If convolution is valid, the **calculations can be accelerated** dramatically. The validity of the convolution relation can be easily verified numerically.

Updates of Core SRW Functions Made at NSLS-II (in collaboration with other Labs)

- Accurate partially-coherent emission and wavefront propagation simulations for SR sources are possible with SRW since ~2009:
  O.Chubar, Y.S.Chu, K.Kaznatcheev, H.Yan, AIP Conf. Proc. Vol. 1234, pp.75-78 (2009)
  O.Chubar, Y.S.Chu, K.Kaznatcheev, H.Yan, Nucl. Instr. and Meth., vol. A649, Issue 1, pp.118-122 (2011)
- Parallel calculations of Partially-Coherent Emission and Wavefront Propagation are implemented in SRW for Python (based on MPI / mpi4py). Besides "normal" Intensity, calculation of Mutual Intensity / Degree of Coherence is possible:
  O.Chubar, A.Fluerasu, L.Berman, K.Kaznatcheev, L.Wiegart, J. Phys.: Conf. Ser. 425, 162001 (2013)
  D.Laundy, J.P.Sutter, U.H.Wagner, C.Rau, C.A.Thomas, K.J.S.Sawhney, and O.Chubar, J. Phys.: Conf. Ser. 425, 162002 (2013)
- Increased reliability of Time- / Frequency-Dependent FEL Pulse Propagation simulations:
  S.Roling, H.Zacharias, L.Samoylova, H.Sinn, Th.Tschentscher, O.Chubar, A.Buzmakov, E.Schneidmiller, M.V.Yurkov, F.Siewert, S.Braun, and P.Gawlitza, Phys. Rev. ST Accel. Beams 17, 110705 (2014)
- New physical-optics "propagators" are implemented for:

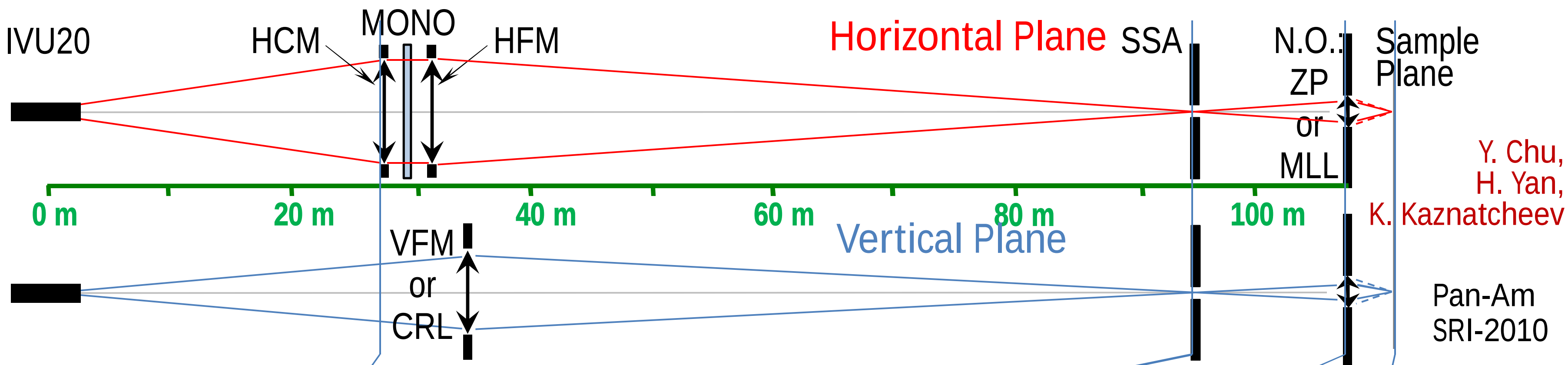
  - Grazing-Incidence Focusing Mirrors, using the stationary phase method / "local ray-tracing":
    N.Canestrari, O.Chubar, R.Reininger, J. Synchrotron Rad. 21, 1110-1121 (2014)

  - Perfect Crystals, using the X-ray Dynamical Diffraction methods:
    J.P.Sutter, O.Chubar, A.Suvorov, Proc. SPIE Vol. 9209, 92090L (2014)
    A.Suvorov, Y.Q.Cai, J.P.Sutter, O.Chubar, Proc. SPIE Vol. 9209, 92090H (2014)

  - Variable Line Spacing Gratings, using the stationary phase method:
    N.Canestrari, V.Bisogni, A.Walter, Y.Zhu, J.Dvorak, E.Vescovo, O.Chubar, Proc. SPIE Vol. 9209, 92090I (2014)

R&D Direction: Improvement of efficiency and reliability of Partially-Coherent “Forward” Simulation

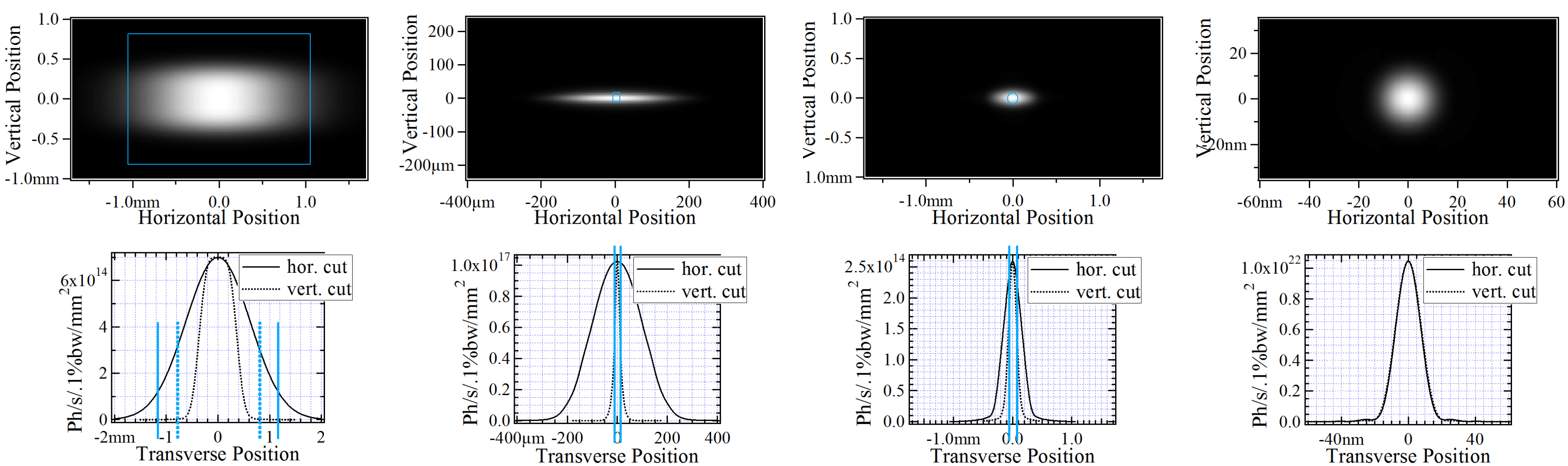
NSLS-II Hard X-Ray Nanoprobe (HXN) Beamline Optical Scheme and Wavefront Propagation Simulation



Flux after HCM: **~7.4x10^{14}** ph/s/.1%bw

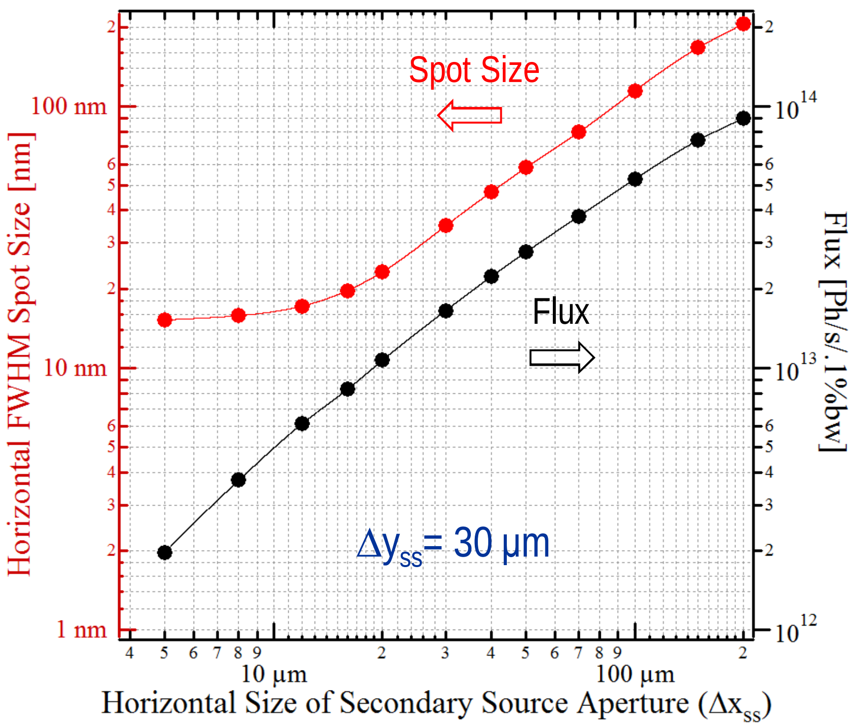
Intensity Distributions

Flux within N.O. Aperture (d=150 µm): **~3.6 x10^{12}** ph/s/.1%bw

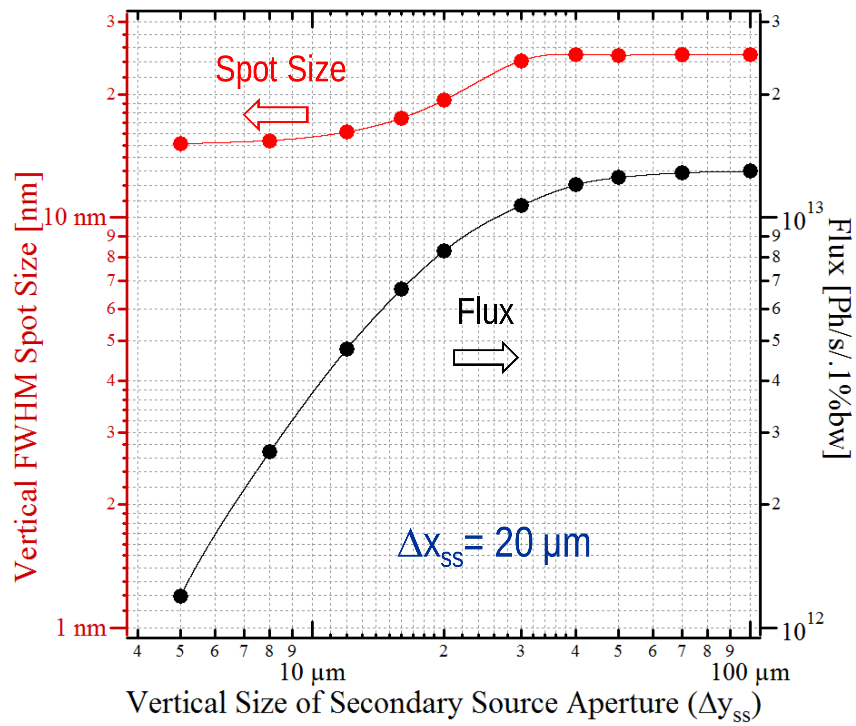


Final Focal Spot Size and Flux at Sample vs Secondary Source Aperture Size (HXN, NSLS-II)

Horizontal Spot Size and Flux
vs Horizontal Secondary Source Aperture Size



Vertical Spot Size and Flux
vs Vertical Secondary Source Aperture Size



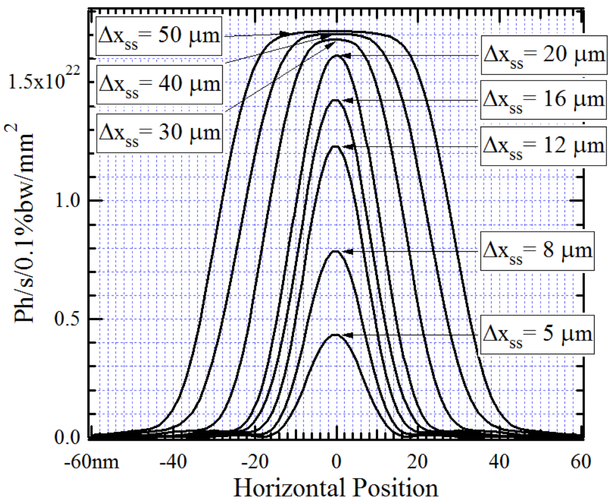
Pan-Am SRI-2010

Secondary Source Aperture located at 94 m from Undulator
Spot Size and Flux calculated for Nanofocusing Optics simulated by Ideal Lens
with F = 18.14 mm, D = 150 μm located at 15 m from Secondary Source (109 m from Undulator)

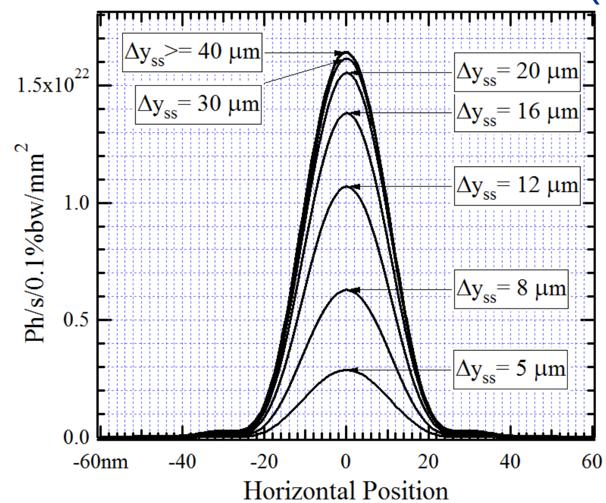
Intensity Distributions at Sample for Different Secondary Source Aperture Sizes at HXN (NSLS-II)

In Horizontal Median Plane (y = 0)

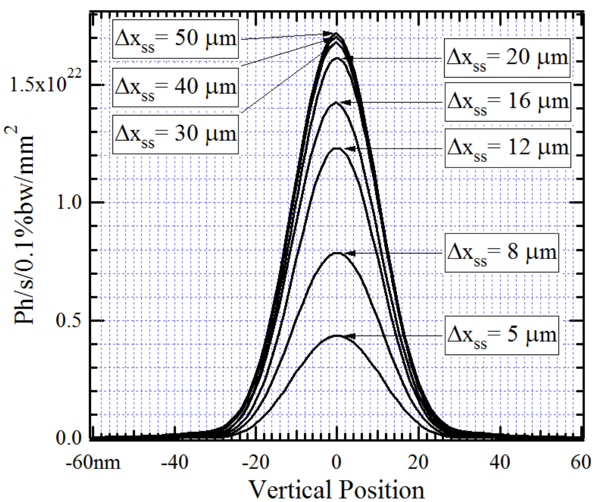
For Different Horizontal SSA Sizes (Δx_{ss})

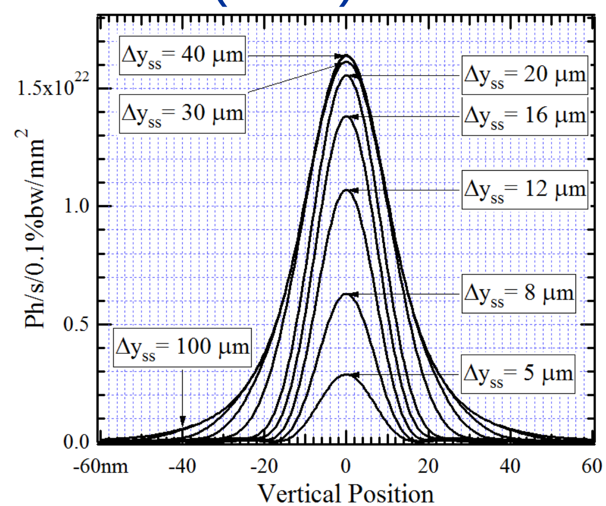


For Different Vertical SSA Sizes (Δy_{ss})



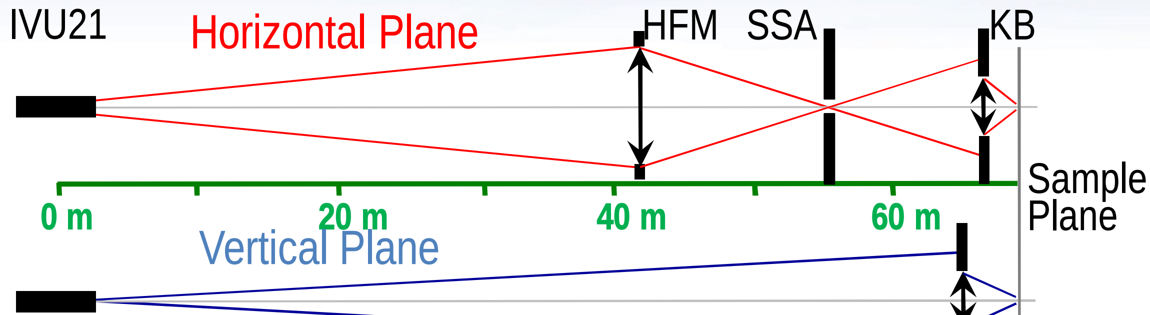
In Vertical Median Plane (x = 0)





For Nanofocusing Optics with F = 18.14 mm, D = 150 μm ($\Delta r \approx$ 15 nm; $E_{ph} \approx$ 10 keV)
SSA located at 94 m, Nanofocusing Optics at 109 m from Undulator

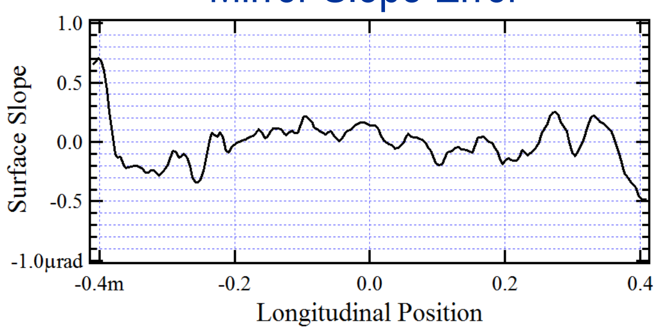
Partially-Coherent Wavefront Propagation Simulations for a Beamline with Grazing-Incidence Focusing Mirrors, Taking Into Account Their Imperfections (FMX @ NSLS-II)



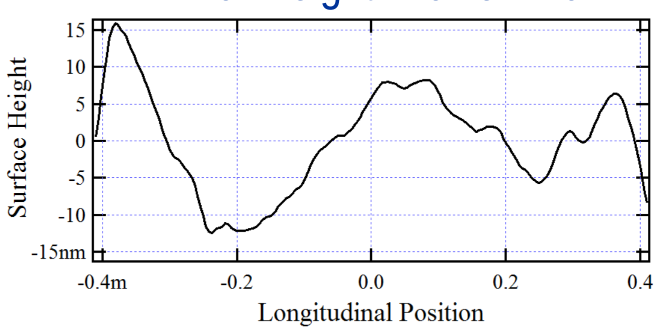
KB simulated using Grazing-Incidence "Thick Optical Element" Propagator based on "Local Ray-Tracing".
KB Surface Height Error simulated by corresponding Phase Shifts ("Masks") in Transverse Plane at Mirror Locations.

Horizontal SSA Size: 30 μm
Photon Energy: 12.7 keV
Flux at Sample: ~5.4x10[13] ph/s/.1%bw

Mirror Slope Error

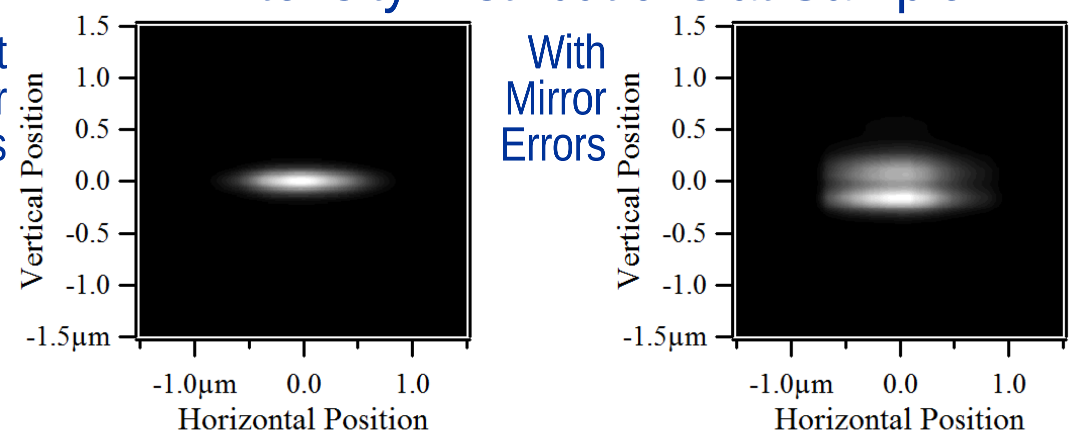


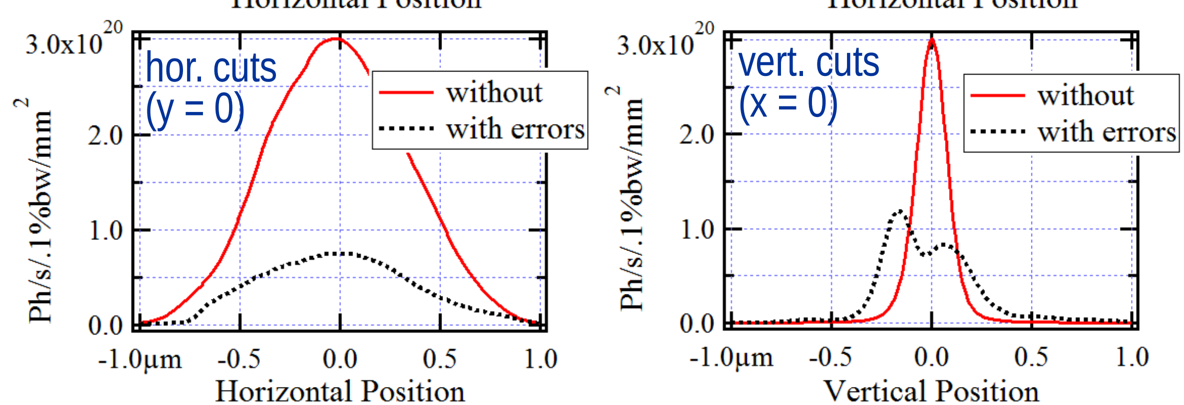
Mirror Height Profile Error



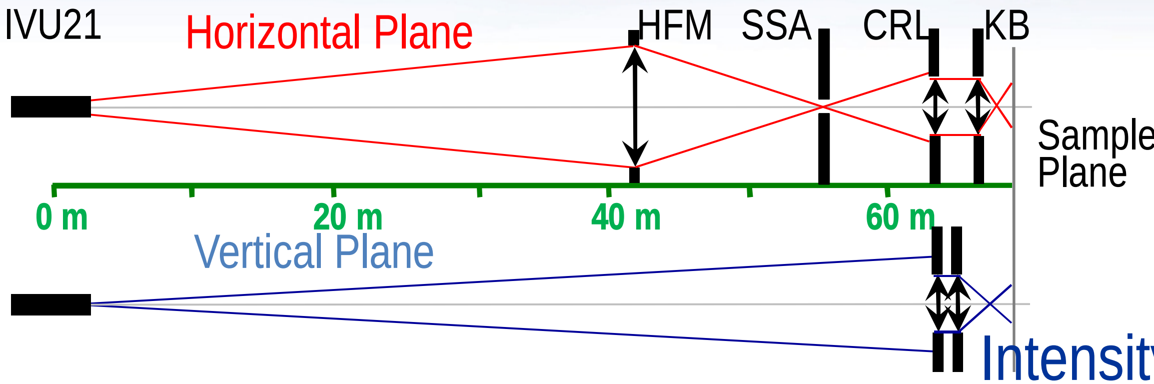
Intensity Distributions at Sample

Without Mirror Errors





Using CRL for Producing “Large Spot” at Sample of FMX Beamline @ NSLS-II



Source:

Electron Current: 0.5 A
Horizontal Emittance: 0.55 nm (“ultimate”)
Vertical Emittance: 8 pm
Undulator: IVU21-1.5 m centered at +1.25 m from Low-Beta Straight Section Center

Horizontal SSA Size: 30 μm
Photon Energy: 12.7 keV

CRL “Transfocator”:

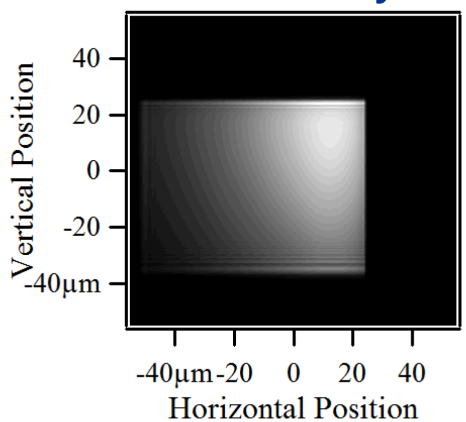
8 Horizontally + **3** Vertically-Focusing Be Lenses
R_{min} = 200 μm
$F_h \approx$ 5.9 m, $F_v \approx$ 15.8 m
Geom. Ap.: 1 mm x 1 mm

Located at 0.75 m before VKB edge
(10 m after SSA)

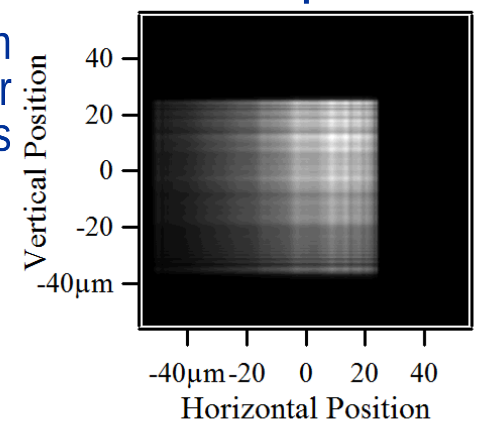
Flux Losses at CRL: ~1.6 times

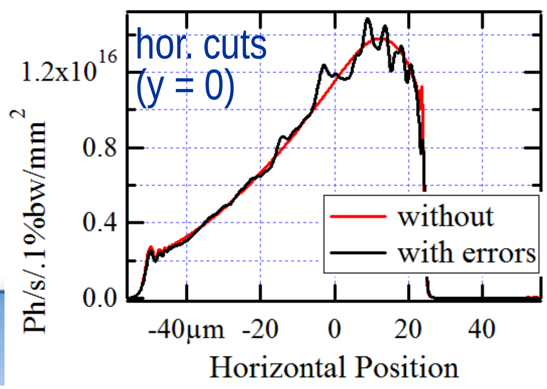
Intensity Distributions at Sample

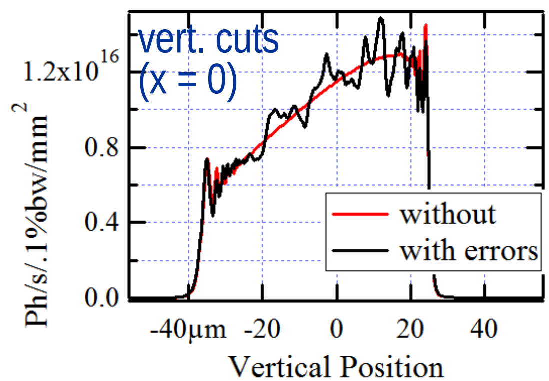
Without Mirror Errors



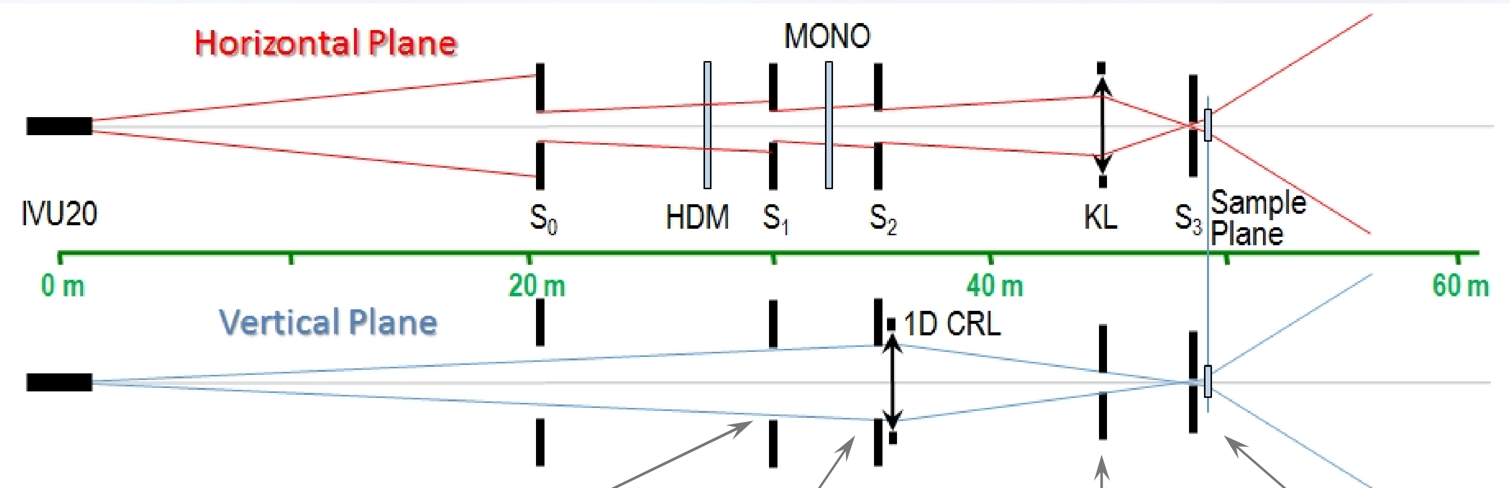
With Mirror Errors







Partially-Coherent Wavefront Propagation Simulations for CHX Beamline @ NSLS-II

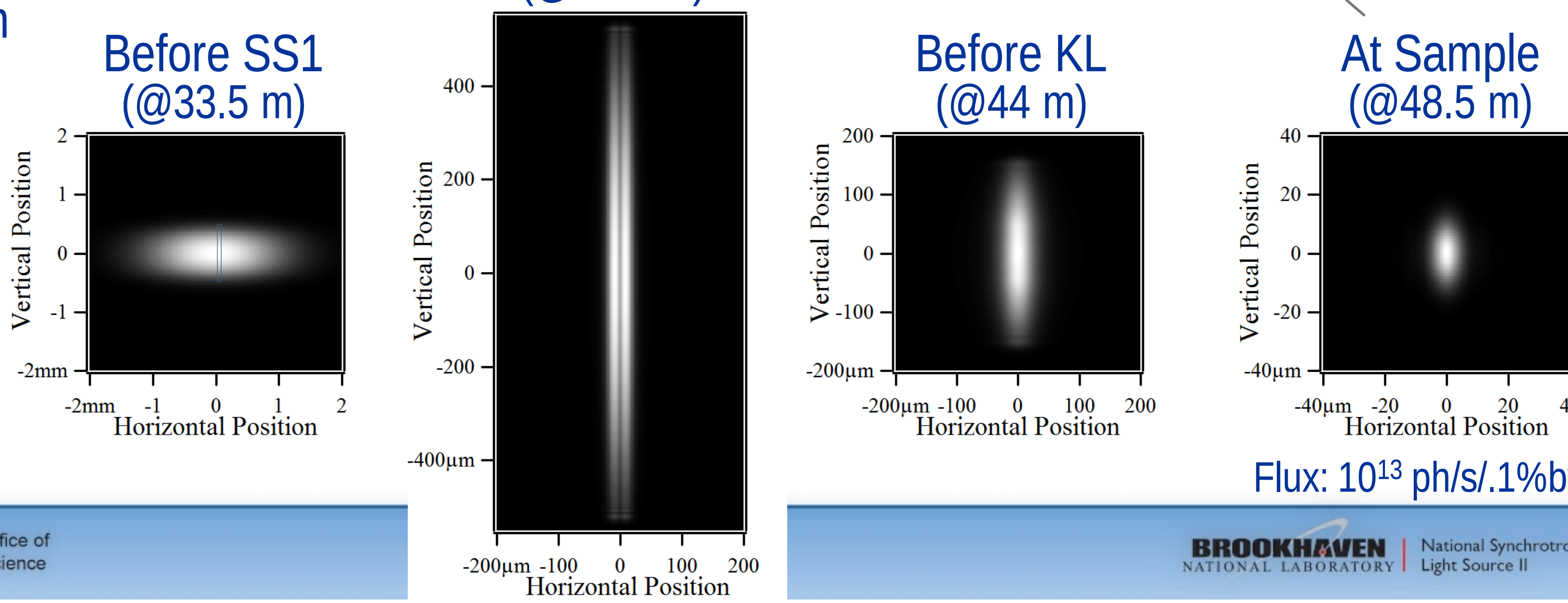


Intensity Distributions

for E = 10 keV

ΔS_{1x}= 44 µm

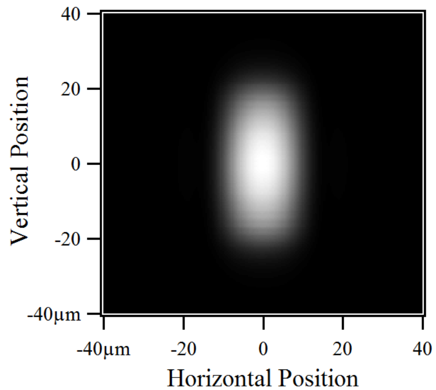
ΔS_{1y}= 1 mm



Flux: 10^{13} ph/s/.1%bw

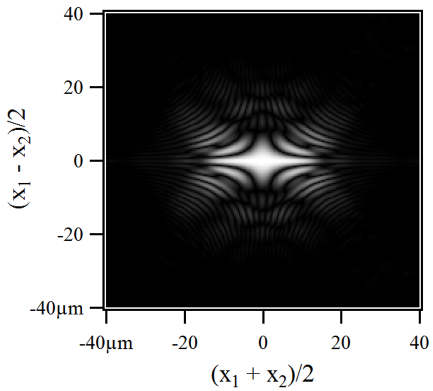
Tracking Intensity and Degree of Transverse Coherence at a Sample (CHX @ NSLS-II)

Intensity Distribution

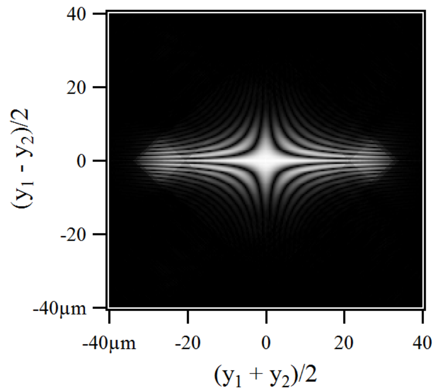


Degree of Transverse Coherence

In Horizontal Mid-Plane



In Vertical Mid-Plane

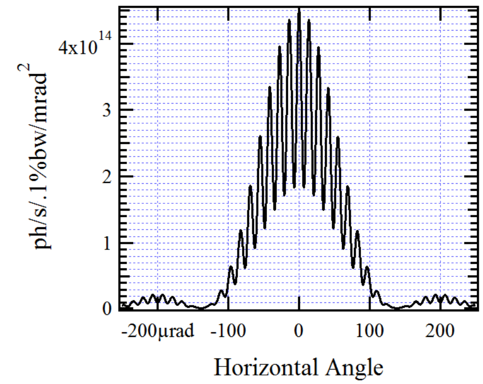


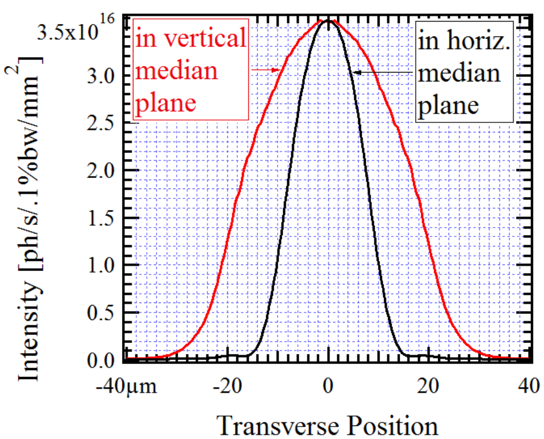
$$\mu(\mathbf{r}_1,\mathbf{r}_2,\omega) = |W(\mathbf{r}_1,\mathbf{r}_2,\omega)|/[W(\mathbf{r}_1,\mathbf{r}_1,\omega)W(\mathbf{r}_2,\mathbf{r}_2,\omega)]^{1/2}$$

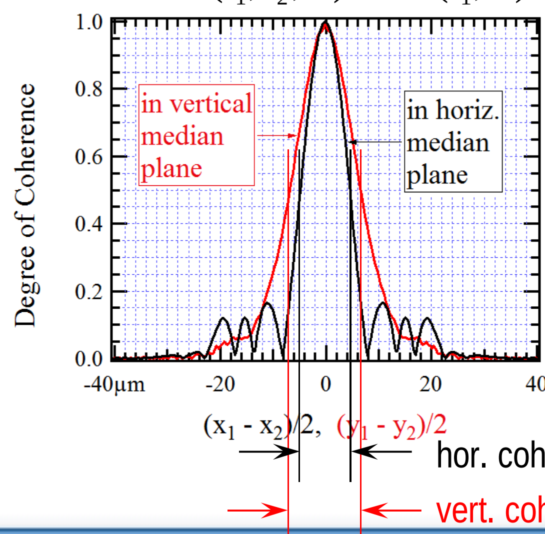
$$W(\mathbf{r}_1,\mathbf{r}_2,\omega) \sim < E(\mathbf{r}_1,\omega)E^*(\mathbf{r}_2,\omega) >$$

Angular Intensity (far field) after Two Slits separated by 10 µm

In Horizontal Plane (after vertical slits)



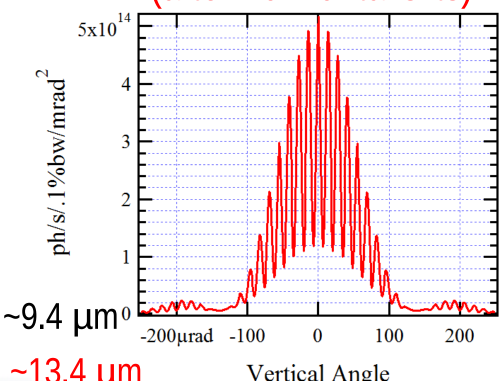




hor. coherence length: ~9.4 µm

vert. coherence length: ~13.4 µm

In Vertical Plane (after horizontal slits)



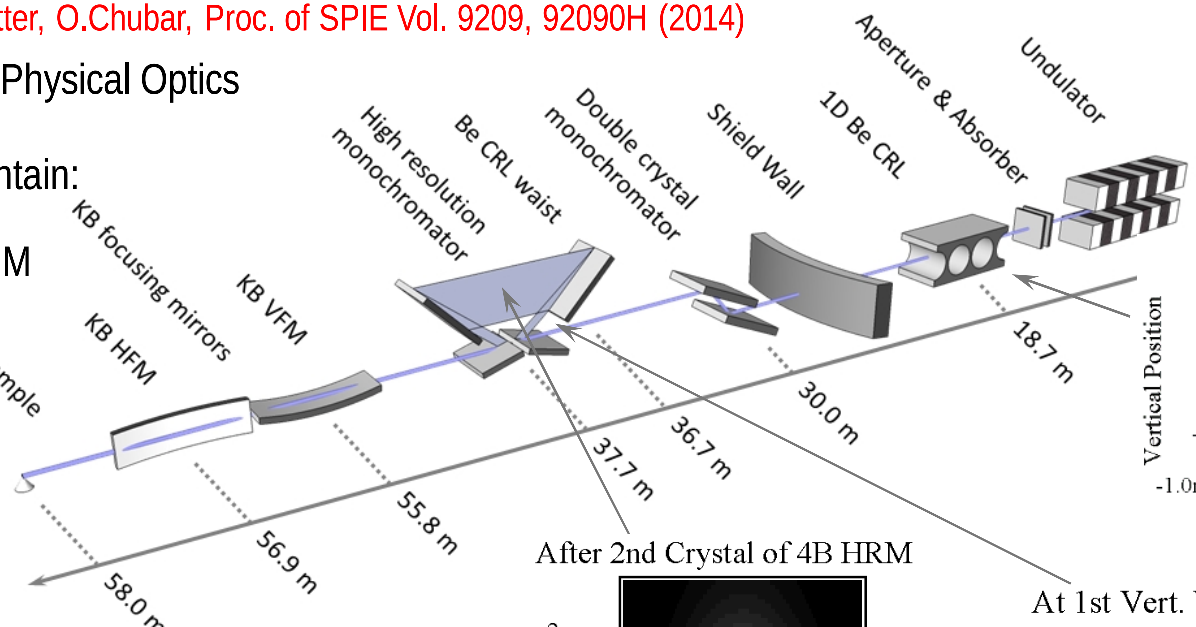
Good agreement with 2-slit interference simulation results

Partially-Coherent Wavefront Propagation Simulations for Inelastic X-ray Scattering Beamline with Advanced High-Resolution Crystal Optics (IXS @ NSLS-II)

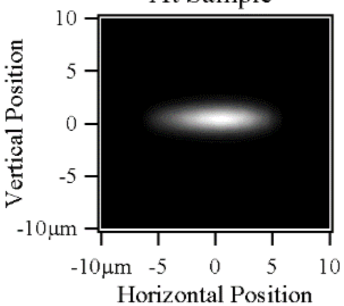
A.Suvorov, Y.Q.Cai, J.P.Sutter, O.Chubar, Proc. of SPIE Vol. 9209, 92090H (2014)

Extended testing of new Physical Optics Propagator for Crystals

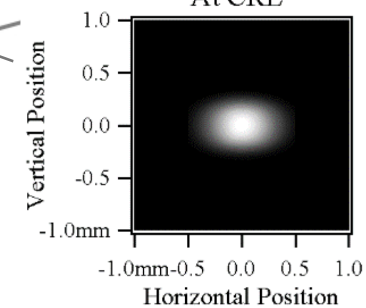
IXS Monochromators contain:
- DCM: 2 Crystals
- HRM: 4 Crystals of HRM



At Sample



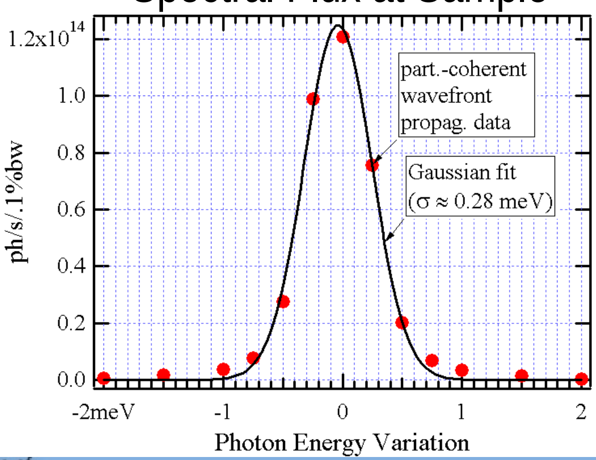
At CRL



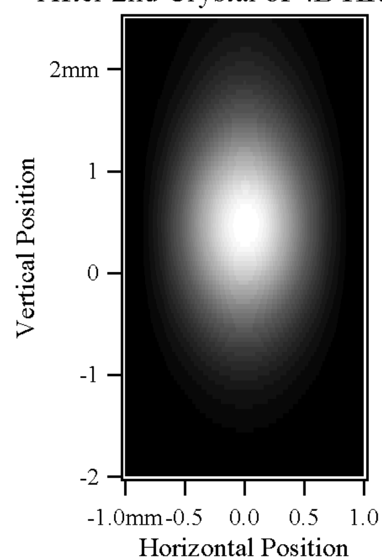
Mirror Surface Error is not taken into account

$E_0 \approx 9131.7$ eV

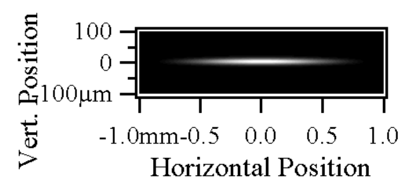
Spectral Flux at Sample



After 2nd Crystal of 4B HRM



At 1st Vert. Waist



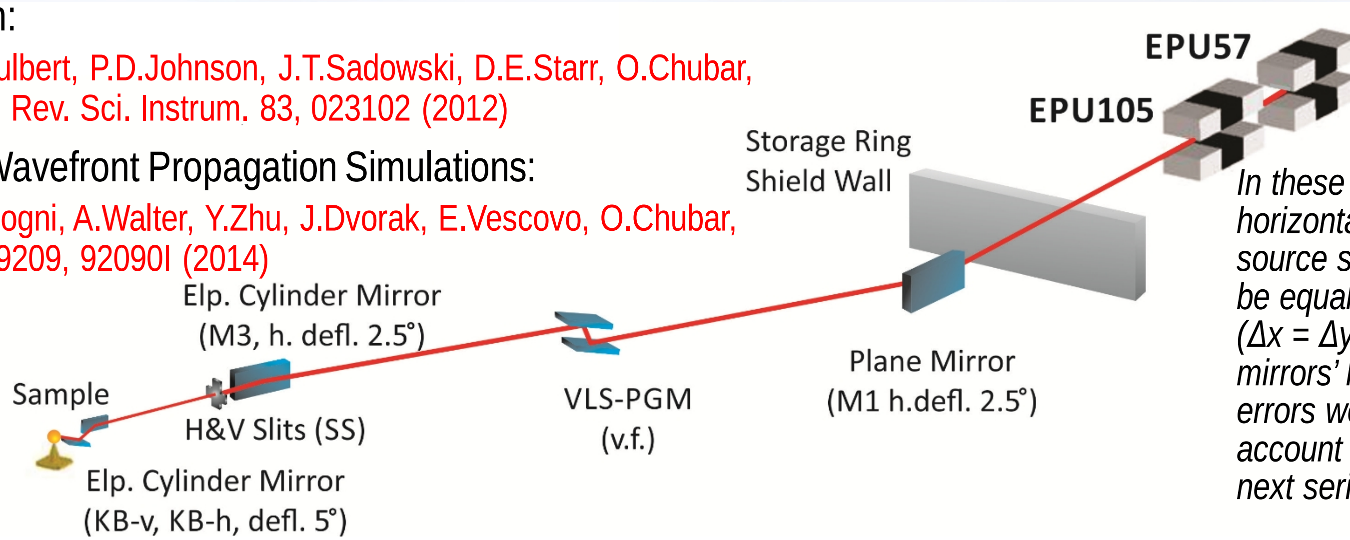
Partially-Coherent Wavefront Propagation Simulations for a Soft X-ray Beamline with VLS grating (ESM @ NSLS-II)

Beamline Design:

R.Reininger, S.L.Hulbert, P.D.Johnson, J.T.Sadowski, D.E.Starr, O.Chubar, T.Valla, E.Vescovo, Rev. Sci. Instrum. 83, 023102 (2012)

Part.-Coherent Wavefront Propagation Simulations:

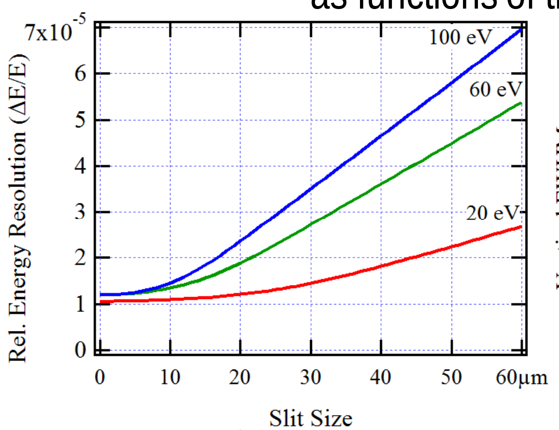
N.Canestrari, V.Bisogni, A.Walter, Y.Zhu, J.Dvorak, E.Vescovo, O.Chubar, Proc. of SPIE Vol. 9209, 92090I (2014)

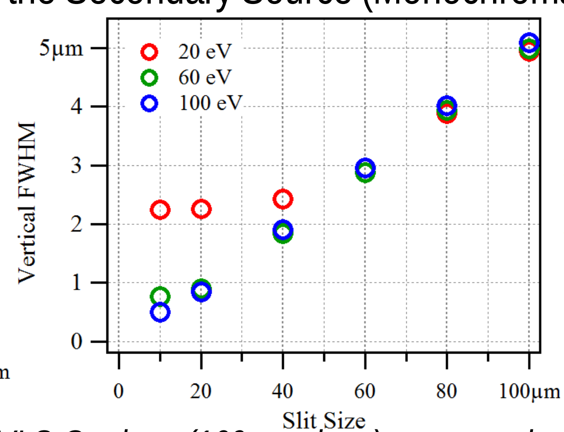


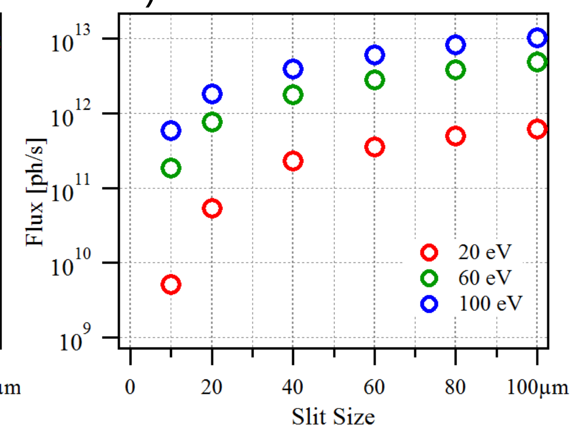
In these simulations, the horizontal secondary source slit size was set to be equal to the vertical size ($\Delta x = \Delta y$); mirrors' height / slope errors were not taken into account (to be included in next series of simulations).

Energy Resolution   Spatial Resolution   Flux (finite-bandwidth) at Sample

as functions of the Secondary Source (Monochromator Exit) Slits







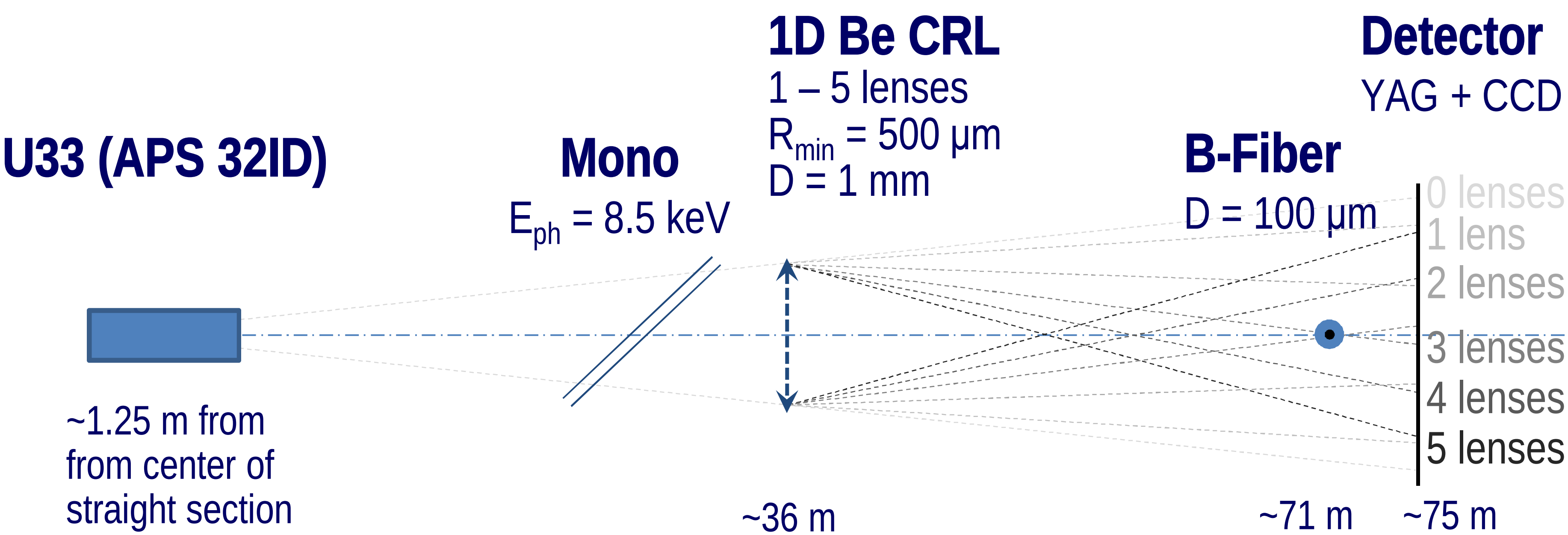
$\Delta E/E > (mN)^{-1}$

Two different VLS Gratings (160 mm long) were used:
a_0= 800 lines/mm for E = 20 eV; a_0= 600 lines/mm for E = 60, 100 eV

Approach to Coherence Preservation Diagnostics Assisted by Simulations (Illustration)

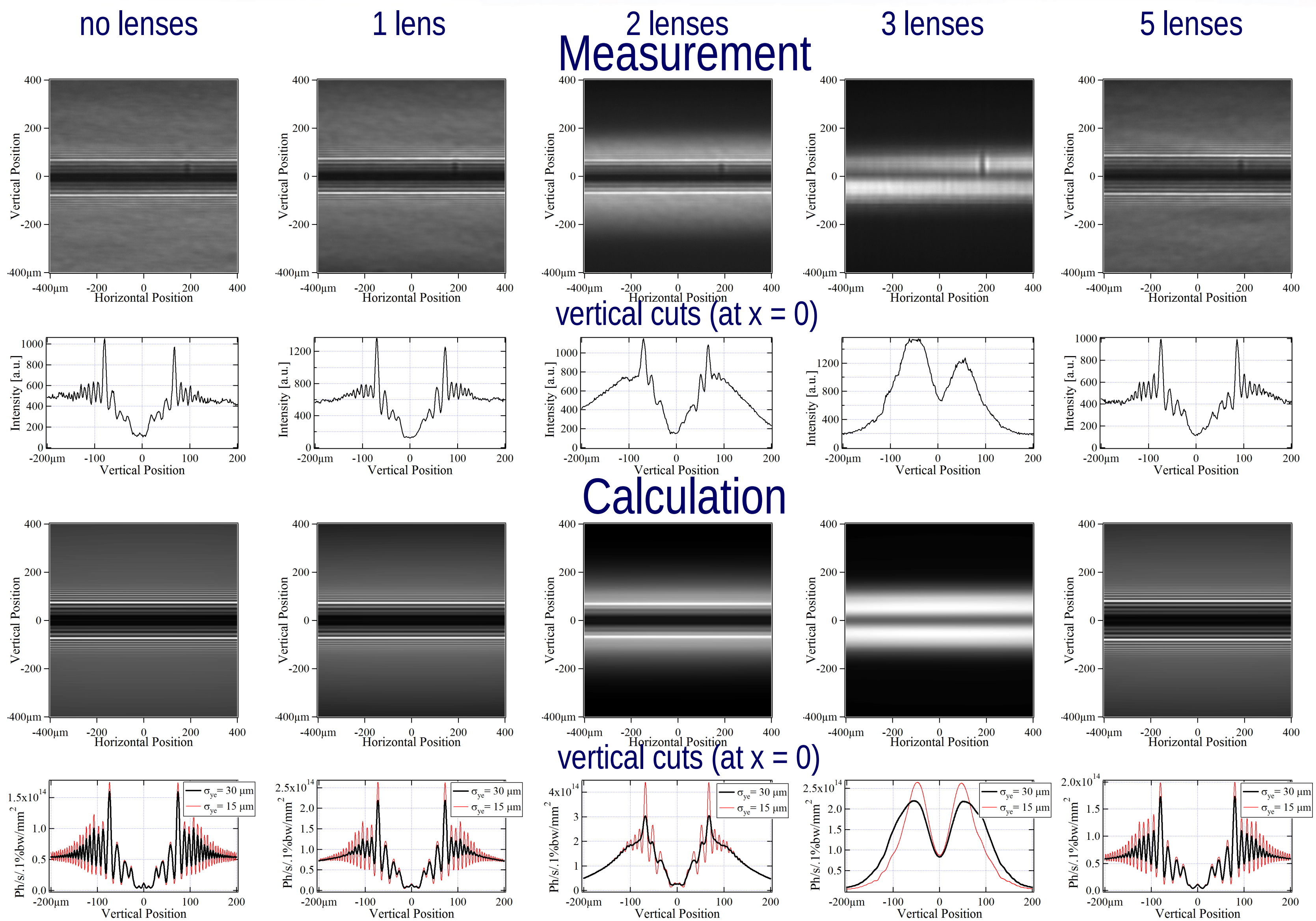
- V.Kohn, I.Snigireva and A.Snigirev, "Direct measurement of transverse coherence length of hard X-rays from interference fringes", Phys. Rev. Lett., vol.85(13), p.2745 (2000)
- A.Snigirev, V.Kohn, I.Snigireva, B.Lengeler, "A compound refractive lens for focusing high-energy X-rays", Nature, vol.384, p.49 (1996)
- O.Chubar, A.Fluerasu, Y.S.Chu, L.Berman, L.Wiegart, W.-K.Lee, J.Baltser, "Experimental characterization of X-ray transverse coherence in the presence of beam transport optics", J. Phys.: Conf. Ser. 425, 052028 (2013)

Optical scheme of test experiments with CRL and a Boron fiber probe



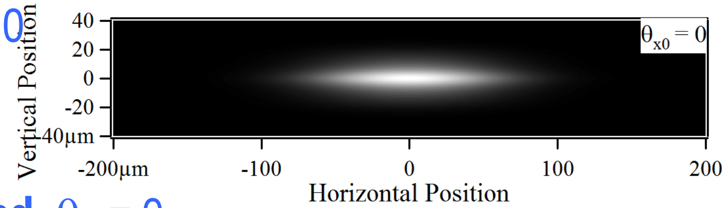
Intensity Distributions in the B-fiber Based Interference Scheme for Different Numbers of CRL in Optical Path

Simulations allow to conclude about coherence preservation in presence of any beamline optics!



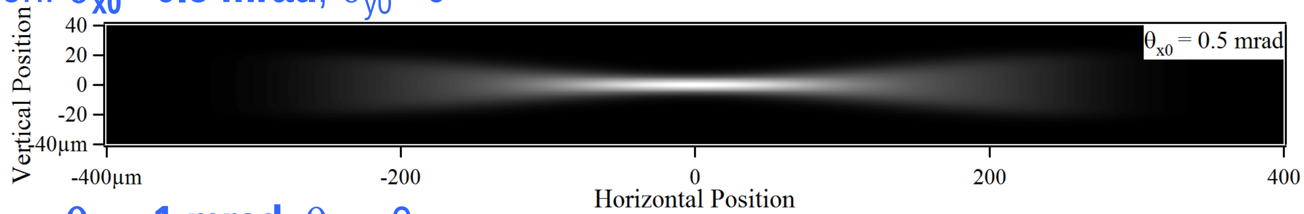
Intensity Distributions of Focused Wiggler Radiation from Partially-Coherent Wavefront Propagation Calculations

On-Axis Collection: $\boldsymbol{\theta_{x0}= 0}$, $\theta_{y0}= 0$
$|\theta_x - \theta_{x0}|< 0.1$ mrad
$|\theta_y - \theta_{y0}|< 0.1$ mrad

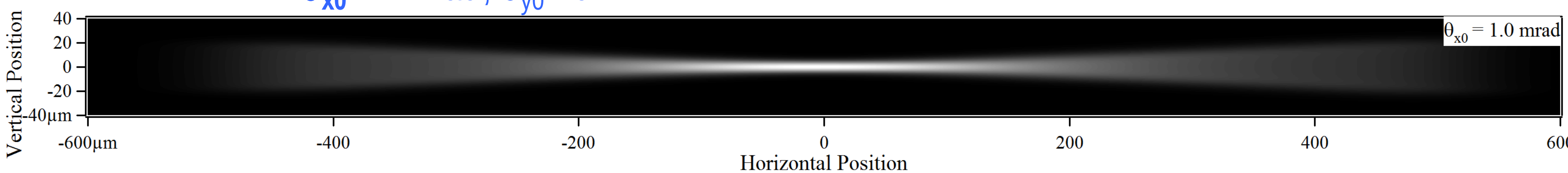


1 : 1 Imaging Scheme with "Ideal Lens"

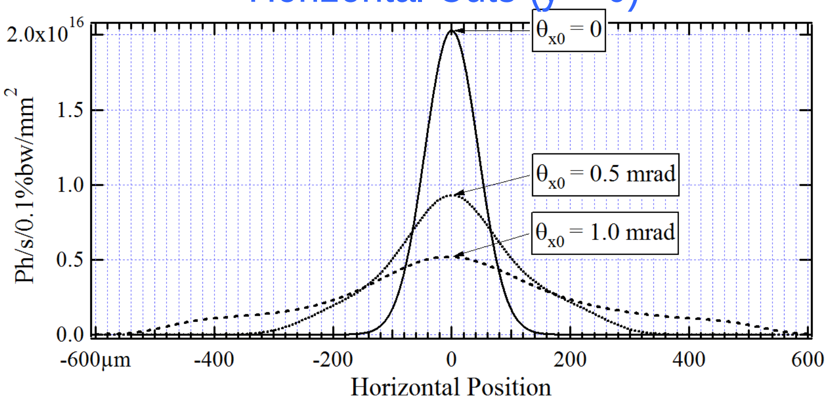
Off-Axis Collection: $\boldsymbol{\theta_{x0}= 0.5}$ **mrad**, $\theta_{y0}= 0$



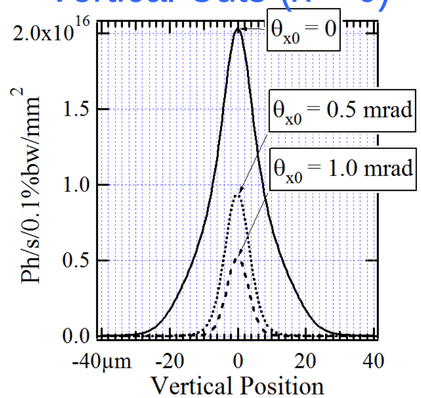
$\boldsymbol{\theta_{x0}= 1}$ **mrad**, $\theta_{y0}= 0$



Horizontal Cuts (y = 0)



Vertical Cuts (x = 0)



NSLS-II Low-Beta Straight Section
$I = 0.5$ A, $\varepsilon_x= 0.9$ nm, $\varepsilon_y= 8$ pm

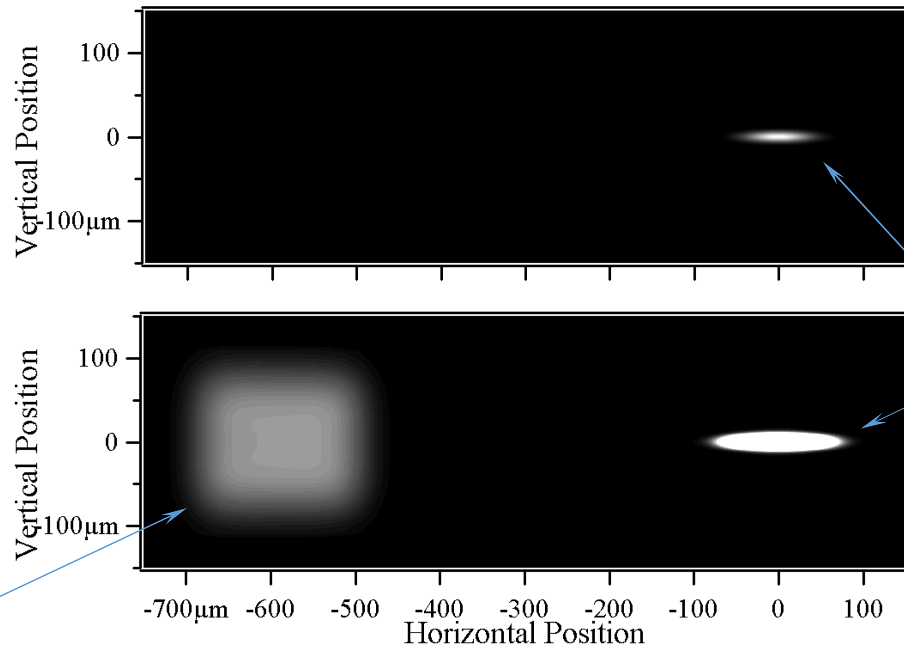
SCW40: $\lambda_u= 40$ mm, $B_{max}= 3$ T, $L = 1$ m
Photon Energy: $E_{ph}= 10$ keV

Intensity Distributions of Monochromatic Radiation from ESRF-U 2PW in 1:1 Imaging Plane

"Non-saturated" Image Plot:

"Saturated" Image Plot:
(max. intensity 50 times lower than in the "non-saturated" plot)

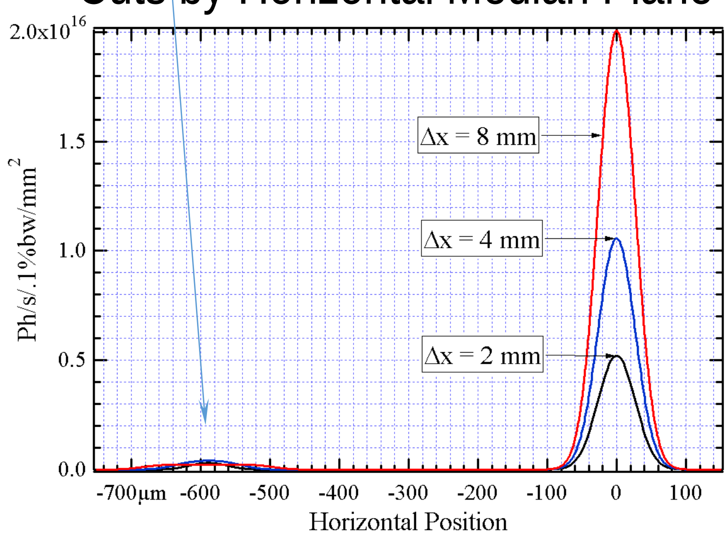
From Downstream Dipole (out of focus)



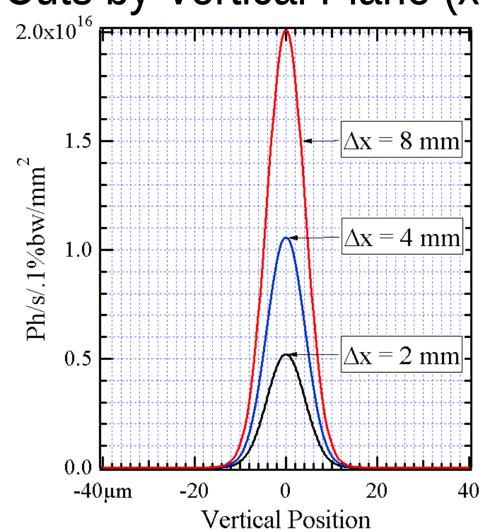
Focusing by Ideal Lens located at: R = 30 m
Lens Aperture:
Δx = 8 mm, Δy = 10 mm
Photon Energy: 5 keV

From 2PW (well focused)

Cuts by Horizontal Median Plane



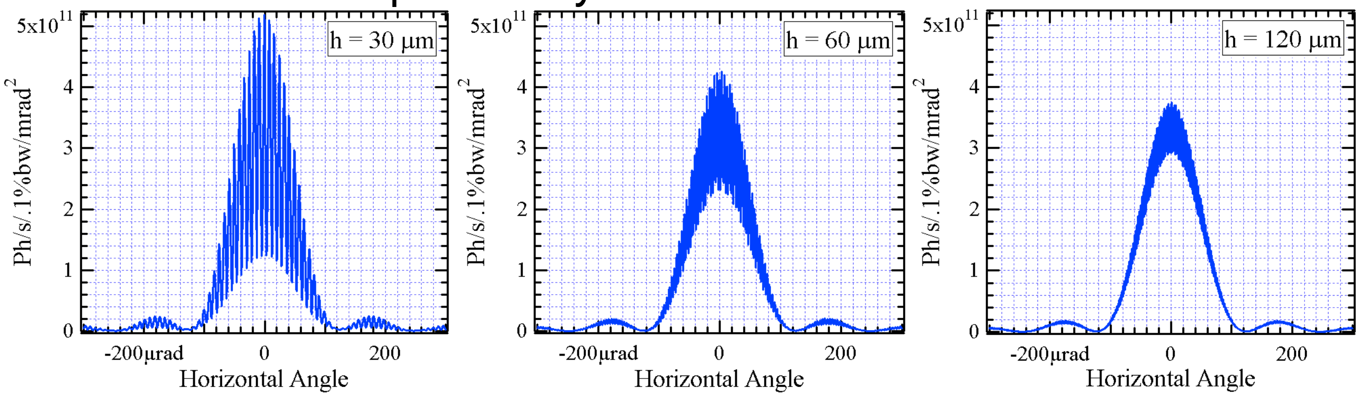
Cuts by Vertical Plane (x = 0)



at Different Horizontal Apertures

Estimating Degree of Coherence (/ Transverse Coherence Lengths) of Radiation from ESRF-U 2PW by Simulating Young's 2-Slit Interference Schemes

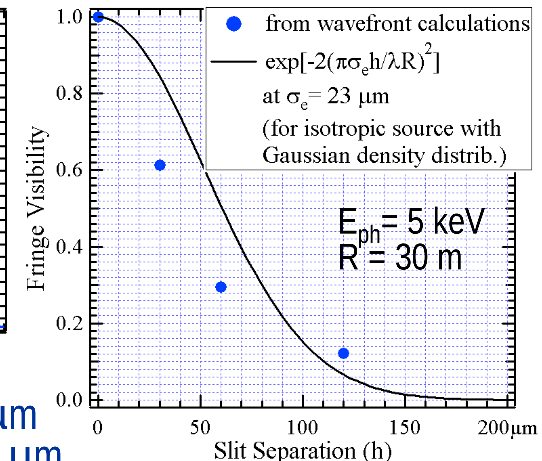
Far-Field Interference Patterns from 2 Vertical Slits Separated by Horizontal Distance h



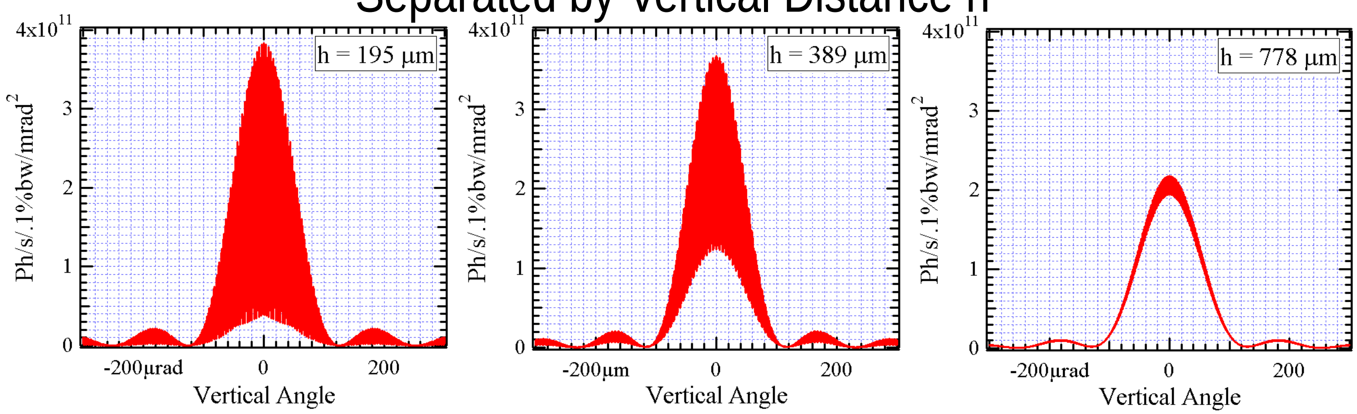
Vertical Aperture: 1 mm; Slit Size: 2 µm

Horizontal Coherence Length: ~40 µm
For a BM-like Source should be ~60 µm

Fringe Visibility vs h in Horizontal Plane



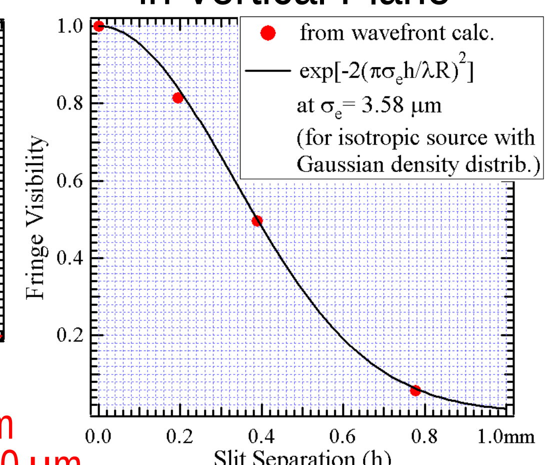
Far-Field Interference Patterns from 2 Horizontal Slits Separated by Vertical Distance h



Horizontal Aperture: 1 mm; Slit Size: 2 µm

Vertical Coherence Length: ~390 µm
For a BM-like Source should be ~390 µm

Fringe Visibility vs h in Vertical Plane



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